WO 2005/120704 PCT/KR2004/001647

CLAIMS

1. A catalyst composition comprising a bidentate ligand represented by formula 1, a monodentate ligand represented by formula 2, and a transition metal catalyst represented by formula 3:

$$R_1$$
 $P - X - Ar_1 - Ar_2 - X - P$ R_2 ...(1)

wherein

5

10

15

20

25

each of R₁ and R₂ is a substituted or unsubstituted C1-20 alkyl group; a substituted or unsubstituted C1-20 alkoxy group; a substituted or unsubstituted C5-20 cycloalkane or cycloalkene; a substituted or unsubstituted C6-36 aryl group; a substituted or unsubstituted or unsubstituted C1-20 heteroalkyl group; a substituted or unsubstituted C4-36 heterocyclic group,

Ar₁-Ar₂ is a bisaryl compound, and X is oxygen (O) or sulfur (S),



wherein

each of R₃, R₄ and R₅ is a substituted or unsubstituted C1-20 alkyl group; a substituted or unsubstituted C1-20 alkoxy group; a substituted or unsubstituted C5-20 cycloalkane or cycloalkene; a substituted or unsubstituted C6-36 aryl group; a substituted or unsubstituted C1-20 heteroalkyl group; a substituted or unsubstituted C4-36 heteroaryl group; or a substituted or unsubstituted C4-36 heterocyclic group, each of R₃, R₄ and R₅ being optionally substituted with nitro (-NO₂), fluorine (F), chlorine (CI), bromine (Br), or a C1-4 alkyl group, and

Y is oxygen (O) or sulfur (S),

$$M(L_1)_1(L_2)_m(L_3)_n$$
 ...(3)

wherein

5

10

15

20

25

M is a transition metal,

each of L_1 , L_2 and L_3 is hydrogen, CO, acetylacetonato, cyclooctadiene, norbornene, chlorine, or triphenylphosphine, and

each of I, m and n is a number of 0 to 5, provided that all I, m and n are not zero simultaneously.

- 2. The catalyst composition of claim 1, wherein in formula 1, each of R_1 and R_2 is pyrrole, phenyl, or indole, and the phosphorous is directly linked to a nitrogen atom.
- 3. The catalyst composition of claim 1, wherein in formula 1, the bisaryl compound Ar_1-Ar_2 is represented by either formula 5 or formula 6:

$$R_{10}$$
 $R_{11}R_{11}$
 R_{10}
 R_{1

wherein

each of R₈, R₉, R₁₀, and R₁₁ is hydrogen, a C1-20 alkyl group, a C6-20 aryl group, a triarylsilyl group, a trialkylsilyl group, a carboalkoxy group, a carboaryloxy group, an aryloxy group, an alkoxy group, an alkylcarbonyl group, an arylcarbonyl group, an amide group, a halogen atom, or a nitrile group, the carboalkoxy group being represented by -CO₂R (wherein R is a C1-20 alkyl group or a C6-20 aryl group),

$$R_{15}$$
 R_{16}
 R_{16}
 R_{17}
 R_{17}
 R_{17}
 R_{18}
 R_{19}
 R_{11}
 R_{12}
 R_{12}
...(6)

wherein

5

each of R₁₂, R₁₃, R₁₄, R₁₅, R₁₆, and R₁₇ is hydrogen, a C1-20 alkyl group, a C6-20 aryl group, a triarylsilyl group, a trialkylsilyl group, a carboalkoxy group, a carboaryloxy group, an aryloxy group, an alkoxy group, an alkylcarbonyl group, an arylcarbonyl group, an amide group, a halogen atom, or a nitrile group, the carboalkoxy group being represented by -CO₂R (wherein R is a C1-20 alkyl group or a C6-20 aryl group).

- 10 4. The catalyst composition of claim 3, wherein in formula 5, R_8 is methyl, methoxy, or t-butyl group, R_9 is hydrogen, R_{10} is methyl, methoxy, or t-butyl, and R_{11} is methyl or hydrogen.
- 5. The catalyst composition of claim 1, wherein in formula 2, Y is oxygen (O), each of R₃, R₄, and R₅ is phenyl, phenyloxy, cyclohexyl, or t-butyl.
 - 6. The catalyst composition of claim 1, wherein in formula 3, the transition metal M is cobalt (Co), rhodium (Rh), or iridium (Ir).
- 7. The catalyst composition of claim 1, wherein the transition metal catalyst is acetylacetonatodicarbonylrhodium (Rh(AcAc)(CO)₂), acetylacetonatocarbonyltriphenylphosphinerhodium (Rh(AcAc)(CO)(TPP)), hydridocarbonyltri(triphenylphosphine)rhodium (HRh(CO)(TPP)₃), acetylacetonatodicarbonyliridium (Ir(AcAc)(CO)₂), or hydridocarbonyltri(triphenylphosphine)iridium (HIr(CO)(TPP)₃).

WO 2005/120704 PCT/KR2004/001647

8. The catalyst composition of claim 1, wherein the concentration of the transition metal is 50 to 500 ppm based on the amount of the catalyst composition, and the concentration of the bidentate ligand is 0.5 to 20 mol and the concentration of the monodentate ligand is 0.1 to 200 mol, respectively, per mol of the transition metal.

5

9. The catalyst composition of claim 1, wherein the transition metal catalyst is acetylacetonatodicarbonylrhodium (Rh(AcAc)(CO)₂), the bidentate ligand is 1,1'-biphenyl-2,2'-diyl-bis(dipyrrolylphosphoramidite) (BPO-P(Pyl)₂), and the monodentate ligand is triphenylphosphine oxide (TPPO).

10

10. A process of hydroformylating an olefin compound, comprising reacting the olefin compound with a gas mixture of hydrogen and carbon monoxide with stirring at elevated pressure and temperature in the presence of the catalyst composition of any one of claims 1 to 9 to produce an aldehyde.

15

11. The process of claim 10, wherein the olefin compound is represented by formula 4:



...(4)

20

wherein

each of R₆ and R₇ is hydrogen, a C1-20 alkyl group, fluorine (-F), chlorine (-Cl), bromine (-Br), trifluoromethyl (-CF₃), or a C6-20 phenyl group substituted with 0 to 5 substituents selected from the group consisting of nitro (-NO₂), fluorine (-F), chlorine (-Cl), bromine (-Br), methyl, ethyl, propyl and butyl.

25

12. The process of claim 10, wherein the olefin compound is a compound selected from the group consisting of ethene, propene, 1-butene, 1-pentene, 1-hexene, 1-octene, and styrene.

30